SECTION 6.0
MODELING TO SUPPORT THE PERMEABLE BARRIER DESIGN

Modeling enables an understanding of the implications of site characterization information and treatability data. Hydrogeologic modeling is conducted for the following reasons:

- Determine an approximate location and configuration for the permeable barrier with respect to the groundwater flow and plume movement.
- Estimate the expected groundwater flow velocity through the reactive cell.
- Determine the width of the reactive cell and, for a funnel-and-gate configuration, the width of the funnel.
- Estimate the hydraulic capture zone of the permeable barrier.
- Determine appropriate locations for performance and compliance monitoring points (discussed in Section 8).
- Evaluate the hydraulic effects of potential losses in porosity (and potential for flow bypass) over the long term.
- Evaluate the potential for underflow, overflow, or flow across aquifers.
- Incorporate the effects of shifts in groundwater flow direction into the design.
- Incorporate site-specific features such as property boundaries, building foundations, buried utilities, etc., into the design.

Appendix B-1 describes the hydrogeologic computer codes that are available to support permeable barrier design. For most practical purposes, commercially available models such as MODFLOW (flow model) and its enhancements are sufficient for the design, although comparable commercial or proprietary models may be used as well.

Geochemical models available for evaluating permeable barriers are described in Appendix C-1. Commercially available models such as PHREEQ are generally sufficient for the purpose. Most available models are equilibrium models, in which reaction kinetics are not incorporated. However, these models can play an important role in understanding the potential for various reactions as the inorganic parameters in the groundwater (e.g., $S0_4$, Ca, etc.) pass through the reactive cell. This relates to issues of media selection and longevity of the barrier.

6.1 HYDROGEOLOGIC MODELING APPROACH FOR DESIGN AND MONITORING OF PERMEABLE BARRIERS

Hydrogeologic modeling can be used at several stages of the permeable barrier technology implementation. This includes the initial feasibility assessment, the site selection, design optimization, design of performance monitoring network, and longevity predictions. The major advantage of constructing a detailed groundwater flow model is that several design configurations, site parameters, and performance and longevity scenarios can be readily evaluated once the initial model has been set up.

Thus the combined effect of several critical parameters can be incorporated simultaneously into one model. Groundwater modeling has been used at most previous permeable barrier installations. In most cases, groundwater flow models have been used in conjunction with particle tracking codes to construct flownets showing travel paths and residence times through the reactive cell. The models are usually set up after laboratory column tests have shown the feasibility of the degradation, and the reaction half-lives and the resulting residence time requirements have been determined.

This section describes the use of models in the evaluation of permeable barrier design and performance. The general requirements of the modeling codes useful for permeable barrier application, a brief overview of the modeling methodology, descriptions of the available codes, and a review of previous modeling studies for permeable barrier design are presented in Appendix B-1.

The two primary interdependent parameters of concern when designing a permeable barrier are *hydraulic capture zone* width and *residence time.* Capture zone width refers to the width of the zone of groundwater that will pass through the reactive cell or gate (in the case of funnel-and-gate configurations) rather than pass around the ends of the barrier or beneath it. Capture zone width can be maximized by maximizing the discharge (groundwater flow volume) through the reactive cell or gate. Residence time refers to the amount of time contaminated groundwater is in contact with the reactive medium within the gate. Residence times can be maximized either by minimizing the discharge through the reactive cell or by increasing the flowthrough thickness of the reactive cell. Thus, the design of permeable barriers must balance capture zone width (and discharge) against the required residence time. Contamination occurring outside the capture zone will not pass through the reactive cell. Similarly, if the residence time in the reactive cell is too short, contaminant levels may not be reduced sufficiently to meet regulatory requirements.

A number of numerical simulations were performed (Battelle, 1996c) to illustrate the design and evaluation of permeable barriers through modeling. The methodology and results of this modeling are described in Appendix B-2 and summarized below.

6.1.1 Modeling Approach for Relatively Homogeneous Aquifers

An illustration of the modeling approach for relatively homogeneous aquifers is presented in Appendix B-2 (Battelle, 1996c). A relatively homogeneous aquifer can be modeled using 2-D versions of flow and particle-tracking codes. At most existing permeable barrier application sites so far, this simplified approach has been used to locate and design the barrier. Permeable barrier features, such as the reactive cell, pea gravel, or funnel walls, can be inserted into the baseline aquifer model as heterogeneities with the appropriate hydraulic conductivities. The hydraulic conductivity of the reactive cell can be estimated based on the particle size of the reactive medium used or, for more certainty, measured through laboratory permeability testing. Design parameters, such as hydraulic capture zone width (feet), residence time within the reactive cell (hours or days), and groundwater discharge through the gate (ft^3/day) can then be estimated for each simulation. The hydraulic capture zone width in each simulation can be determined by tracking particles forward through the gate.

Figure 6-1 shows the particle tracking result for a permeable barrier in a relatively homogeneous aquifer. The hydraulic capture zone is symmetrical and extends beyond the width of the gate. Remixing of the water flowing through the gate and water flowing around the barrier takes place downgradient. This type of modeling is a useful tool for designing the dimensions of the reactive cell (gate) and funnel, as well as simulating scenarios for different configurations. For example, the funnel walls could be eliminated in one simulation or the width of the reactive cell (gate) could be increased in another simulation.

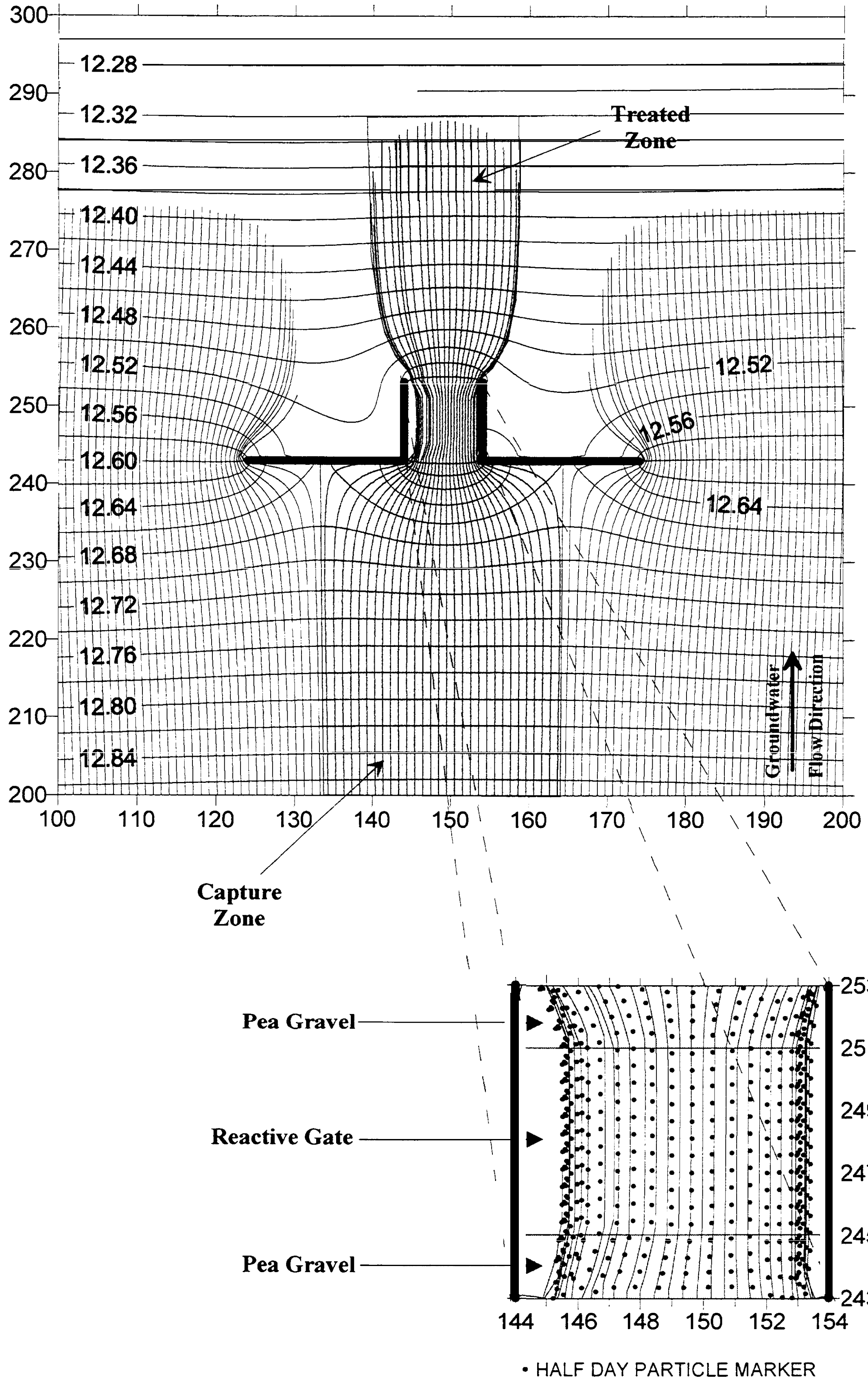

Figure 6-1. Simulated Particle Pathlines Showing Capture Zone

Particle-tracking codes also can be used to design a performance-monitoring network along specific flow paths for evaluation of potential contaminant breakthrough or bypass. This approach is especially useful if tracer tests are to be used to evaluate permeable barrier performance.

6.1.2 Modeling Approach for Heterogeneous Aquifers

Modeling studies and barrier design at most existing permeable barrier sites so far have been primarily based on the assumption that the aquifer sediments in the vicinity of the permeable barrier are homogeneous. However, at many sites, there may be strong heterogeneity in the sediments. This heterogeneity develops mainly due to the variations in depositional environments of the sediments. The general implications of heterogeneity are that more detailed site characterization is required and the models are more complex. The symmetrical capture zones seen in homogeneous sediments become asymmetrical and difficult to predict without detailed characterization and modeling.

Figure 6-2 shows the results of modeling conducted at a permeable barrier site in California (Battelle, 1996c; and PRC, 1996). The capture zones at this site, as seen from these particle tracking maps, are highly *asymmetrical.* In the less-permeable layers (Layers 1 and 2), there is hardly any movement of particles over 25 days. In the more-permeable Layer 3, the particle movement is very fast upgradient of the gate but very slow upgradient of the funnel walls. In the more-permeable Layer 4, the particle movement is very fast in front of the west funnel wall but somewhat slower on the east side. These irregularities exist because the lower part of the permeable barrier (Layers 3 and 4) is in a high-conductivity sand channel, whereas the upper part is located in lower-conductivity interchannel deposits. The location of the sand channels at the site was determined based on existing base-wide site characterization maps and from localized CPT data generated during additional site characterization activities conducted to aid the design of the barrier. The irregularities in flow may result in vastly different residence times in the reactive cell. Pea gravel sections along the upgradient and downgradient edges of the reactive cell help to homogenize the flow vertically and horizontally to some extent.

A similar situation is reported by Puls et al. (1995) for the Elizabeth City, North Carolina, site. At this site the geology is characterized by complex and variable sequences of surficial sands, silts, and clays. Groundwater flow velocity is extremely variable with depth, with a highly conductive layer at roughly 12 to 20 feet below ground surface. The reactive cell was emplaced in this sand channel (see figure in Appendix B-2).

These examples illustrate the need for placing the reactive cell in a zone of high conductivity that forms a preferential pathway for most of the flow and contaminant transport through the aquifer. Additionally, the dependence of capture zones on aquifer heterogeneities illustrates the need for detailed site characterization and adequate hydrogeologic modeling prior to permeable barrier design and emplacement. Particle tracking simulations, such as the one shown in Figure 6-2, along with a flow model based on good site characterization, can also help in optimizing monitoring well locations for evaluating the performance of the barrier.

6.1.3 Modeling Different Permeable Barrier Configurations and Dimensions

One of the advantages of groundwater modeling is that numerous different configurations of the permeable barrier systems can be simulated to select the design most suitable for a site. Thus relative benefits and limitations of various options may be evaluated prior to expensive field installations. Simulation of one of the common designs, the simple funnel-and-gate system, has already been presented in this chapter and in Appendix B-2. In addition, another simulation incorporating a funnel-and-gate design

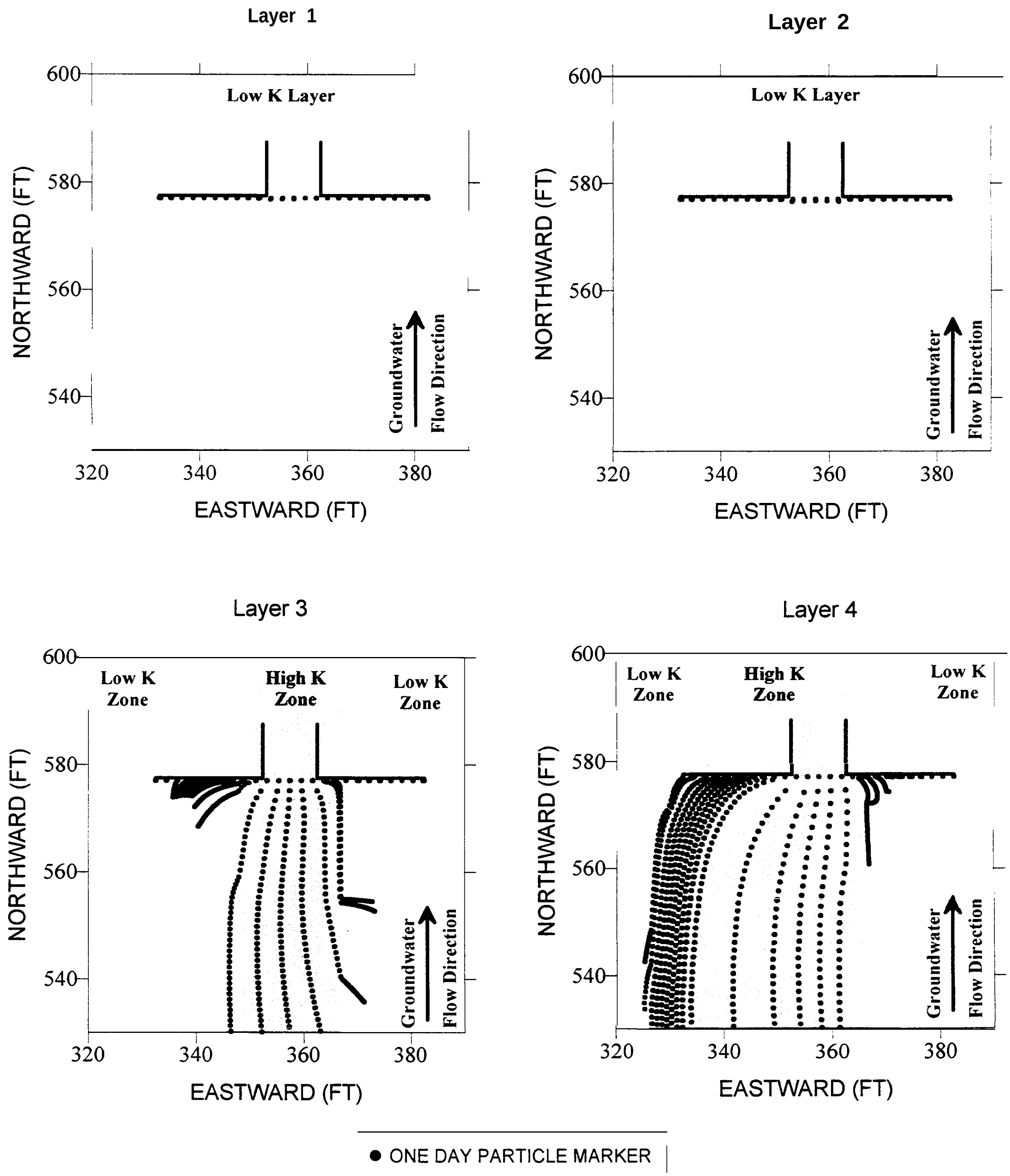

Figure 6-2. MFA Funnel-and-Gate Backward Particle Tracking Showing the Effect of Heterogeneity on Capture Zones (Battelle, 1996c)

in heterogeneous media is shown in Figure 6-2. In this section, two more design scenarios are presented to illustrate the use of groundwater flow models in designing and optimizing permeable barriers (Battelle, 1996c).

An example simulation of the first scenario with a continuous barrier is shown in Figure 6-3. This simulation consists of a 10-foot-long section of reactive media having a 6-foot thickness in the direction of flow. The aquifer is simulated as a single layer having uniform hydraulic properties with a conductivity of 10 feet per day. The reactive media is simulated with a hydraulic conductivity of 283 feet per day. The flow field was simulated with a gradient of 0.005 feet/foot. Particle tracking techniques were used to delineate the capture zone of the reactive media by delineating flow paths for

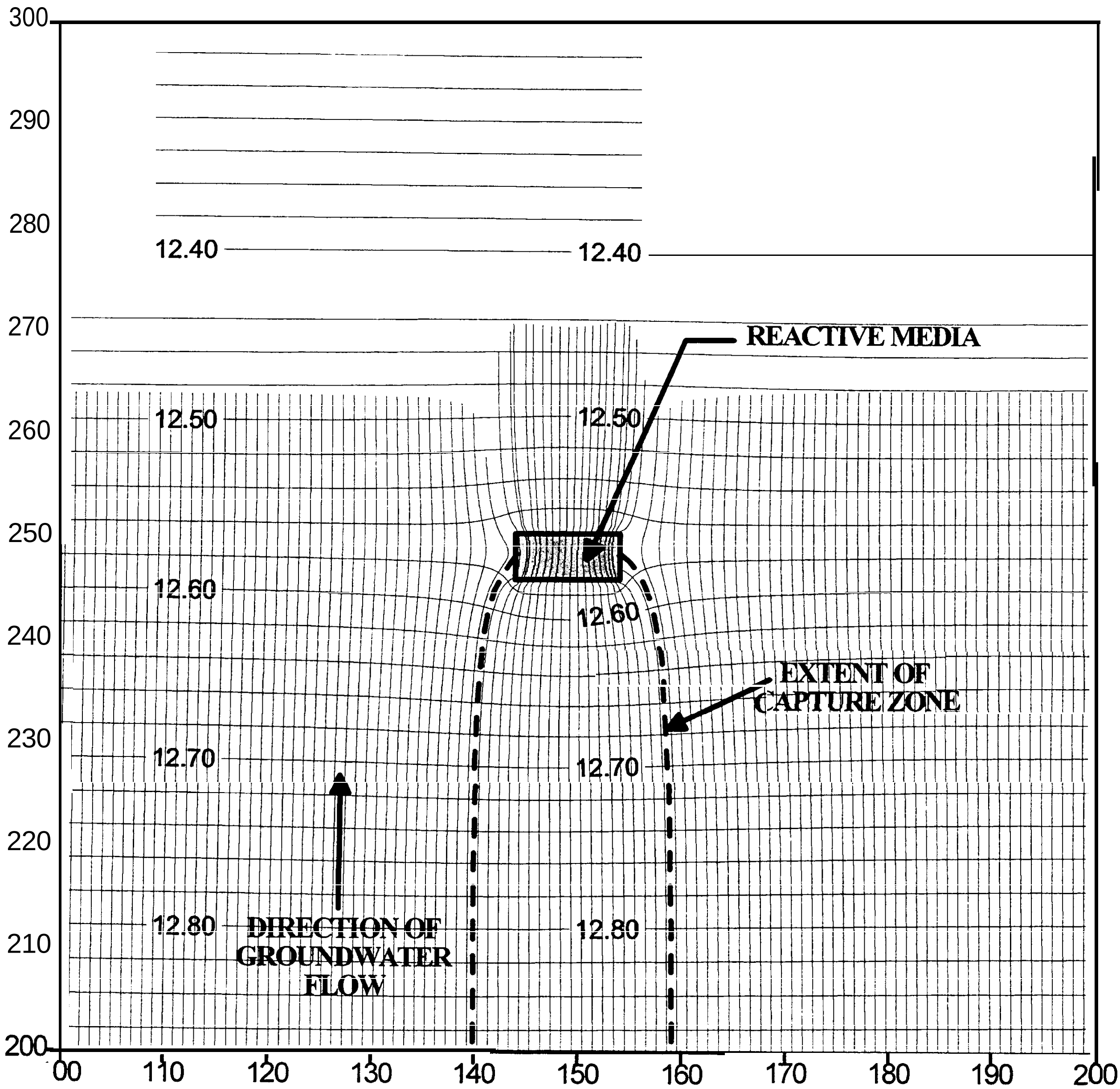

Figure 6-3. Simulated Capture Zone for a Continuous Barrier Scenario Showing Flowpaths for 180 Days

180 days. As indicated by the dashed lines, the capture zone has a width greater than the 10-foot length of the reactive media. The width of the capture zone will increase or decrease as the ratio of the reactive media hydraulic conductivity to the aquifer hydraulic conductivity increases or decreases, respectively. Residence time through the reactive media can be estimated using particle tracking methods to ensure sufficient residence time for the degradation reactions to occur. In this case, where no funnel walls are used, several short flow paths into and out of each end of the reactive media occur. Groundwater flowing along these paths do not pass through the entire thickness of the reactive media, and therefore, entrained contaminants may not be fully degraded in these instances unless appropriate safety factors are incorporated into the design.

The second scenario involves simulation of a permeable barrier with two 8-foot-diameter caissons containing reactive media installed in a funnel-and-gate type configuration similar to that shown in Figure 2-1d. Slurry walls were selected as the materials to be used to construct the funnel walls. A 4-foot by 4-foot zone within the caissons represents the area for the reactive media emplacement. Both up- and downgradient pea gravel are simulated for the areas immediately adjacent to the reactive media. The slurry walls extend 89 feet between the two gate locations and 33 feet on each end of the installation. A single layer, 2-D groundwater flow model was used with the aquifer assumed to have a uniform hydraulic conductivity of 8.5 ft/day. The reactive media was assigned a K of 283 ft/day; pea gravel K = 2,830 ft/day, and slurry walls K = 2.0e-06 ft/day. A gradient of 0.002 was imposed upon the flow system resulting in groundwater flow velocity of about 0.05 ft/day. The calculated flow field was used to estimate the capture zones (Figure 6-4) for the simulated caisson-and-gate installation. Particle tracking techniques using RWLK3D were employed to delineate the flowpaths for 5,000 days. As seen in Figure 6-4, the capture zones for this homogeneous system are roughly symmetrical with flow divides at the approximate midpoints of the funnel walls. However, in heterogeneous systems these capture zones are likely to be asymmetrical. Another noteworthy aspect of this illustration is that it is taking about 10 years for 200 feet of plume capture. This indicates that at low groundwater velocity sites, the remediation of large plumes can take a very long time. At sites such as this, it may be useful to consider using recharge wells upgradient of the permeable barrier to increase hydraulic gradient to accelerate the plume capture.

Models similar to those shown in this section can be set up to evaluate several designs under site-specific conditions before selection of an appropriate design for the final installation. It should be noted that the scenarios presented above are based on highly simplified and idealized situations. For models based on field conditions, it is critical to incorporate heterogeneities, seasonal variations in flow conditions, potential vertical flow gradients, site features such as buried utilities and buildings, and calibration into the model for realistic prediction.

Interrelated with the modeling of different permeable barrier configurations is the modeling of different *dimensions* of the barrier for a given configuration. Different widths of a continuous reactive barrier, gate, or funnel can be simulated to evaluate any trade-offs that may occur between various design parameters (e.g., hydraulic capture zone width versus residence time in the reactive cell.). For example, the illustrative modeling scenarios in Appendix B-2 provide the following considerations for permeable barrier design.

- While designing the dimensions of the reactive cell, it is important to note that $K_{aquifer}$ is the sensitive parameter for discharge and residence time through the reactive cell when the ratio of K_{cell} to $K_{aquifer}$ is greater than 5 to 1. Reductions in K_{cell} do not significantly impact discharge and residence times through the gate until the ratio of K_{cell} to $K_{aquifer}$ drops below 5:1, where K_{cell} becomes an increasingly

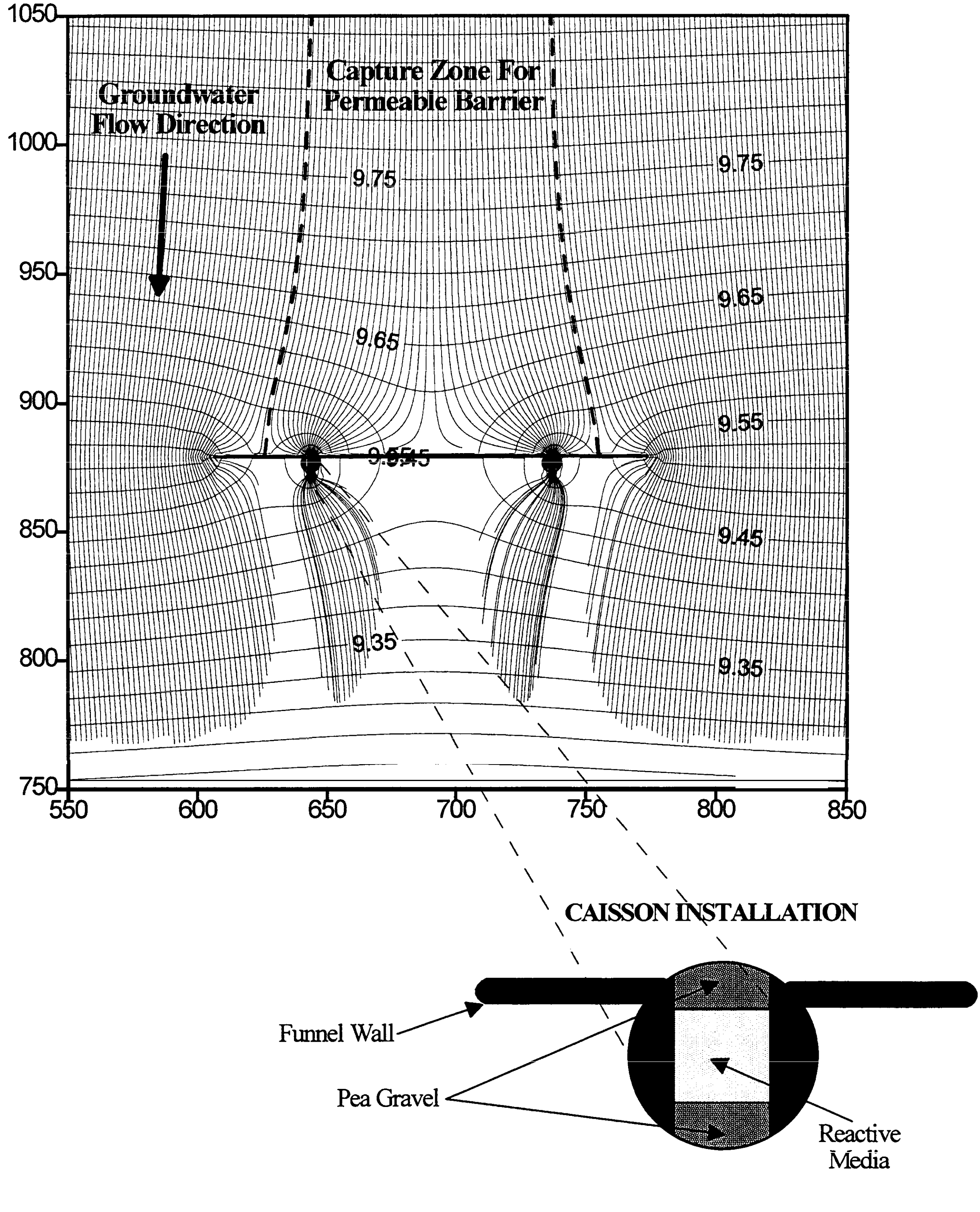

Figure 6-4. Capture Zone for a Permeable Barrier with Two Caissons and Funnel Walls. Flowpaths for 5,000 Days Shown

sensitive parameter. This type of analysis can be used with site-specific models to evaluate the effect of decreasing reactive cell permeability over time on the performance of the permeable cell. Appropriate safety factors (in terms of additional reactive cell width or larger particle size reactive medium) then can be incorporated into the design for anticipated changes in capture zone and residence time.

- As discharge through the reactive cell increases, capture zone width increases, and travel time through the reactive cell (residence time) decreases. For the *scenarios* simulated in this report, residence times in the reactive cell ranged from over 200 days for low-K (0.5 foot/day) aquifers to roughly one day for higher conductivity aquifers (100 feet/day). The estimates of residence times based on the particle tracking can be used to optimize the flowthrough thickness of the reactive cell required for achieving the desired reduction in contaminant levels.

- Particle tracking may also be used to design a performance monitoring network along specific flowpaths. This approach is especially useful if tracer tests are to be conducted in the reactive cell or its vicinity. Some particle tracking codes, such as RWLK3D, can also incorporate the solute transport processes. These may be used to evaluate the effects of dispersion within the reactive cell. The fastest travel times determined from the advective-dispersive simulations would then be used to determine the safety factor required in designing the reactive cell.

- For funnel-and-gate configurations, hydraulic capture zone width appears to be most sensitive to funnel length and aquifer heterogeneity. Capture zone width is generally greater for higher values of K_{cell} when $K_{aquifer}$ is held constant. At ratios greater than 5:1 between K_{cell} and $K_{aquifer}$, capture zone width did not change significantly when only the K_{cell} was varied. Higher conductivity aquifers have larger capture zones relative to less conductive aquifers for the same K_{cell}. Capture zone width is more sensitive to variability in $K_{aquifer}$ relative to changes in K_{cell}.

Similarly, the following design considerations were obtained form the previous modeling studies (Starr and Cherry, 1994; Shikaze, 1996) described in Appendix B-1:

- In a funnel-and-gate configuration, the maximum absolute discharge (groundwater flow volume) through the gate occurs when the funnel walls are at an apex angle of 180 degrees (straight barrier).

- For all apex angles, the maximum discharge occurs when the funnel is perpendicular to the regional flow gradient.

- A balance between maximizing the hydraulic capture zone size of the gate and maximizing the residence time in the reactive cell should be achieved through modeling. In general, for a funnel-and-gate system, hydraulic capture zone size (or discharge through the gate) and residence time are inversely proportional. The residence time can usually be increased without affecting the size of the capture zone by increasing the width of the gate.

- For funnel walls at 180 degrees (straight barrier), the hydraulic capture zone size (or discharge) increases with increasing funnel width. However, the relative capture zone width decreases dramatically as the funnel width increases. The relative capture zone width is the ratio of the capture zone width to the total width of the funnel-and-gate system.

- For a constant funnel width, the absolute and relative capture zone width increase with gate width. Therefore, it is desirable to have a gate as wide as is economical.

- For a given funnel-and-gate design, the capture zone size increases with increase in K_{cell} relative to the aquifer. However, there is relatively little increase in capture zone size when the K_{cell} is more than 10 times higher than $K_{aquifer}$. Therefore, in selecting the particle size of the reactive medium, it is useful to note that the resulting K_{cell} need not be more than about 10 times higher than the K of the surrounding aquifer.

6.2 GEOCHEMICAL EVALUATION FOR PERMEABLE BARRIER DESIGN AND PERFORMANCE

Geochemical modeling is a relatively underutilized area for application to permeable barrier settings. Most designs and performance evaluations have relied more on empirical evidence of reactions between groundwater inorganic parameters (e.g., Ca, Mg, alkalinity) and the reactive medium (iron). One reason for this is possibly the limited availabilities of kinetic geochemical models. Appendix C-1 describes the various geochemical models available and their potential for application to permeable barrier settings. Appendix C-2 illustrates how some of these models can be applied to learn about potential reactions and species formation on the reactive cell.

Geochemical modeling is an attempt to interpret or predict the concentrations of dissolved species in groundwater based on assumed chemical reactions. Early efforts were concerned with performing speciation calculations on dissolved inorganic constituents. The models that were developed as an outgrowth of these efforts can be grouped as forward and inverse models.

In *forward modeling,* reaction progress is governed by thermodynamic expressions, hence the result is an equilibrium prediction. In *inverse modeling,* probable reactions are calculated based on the information supplied at initial and final points along a flowpath, and as such, do not necessarily represent equilibrium. The third type, *reaction-transport modeling,* couples forward modeling with fluid flow and solute transport. This is the newest area of geochemical modeling research, and few highly sophisticated codes have been developed in this area. Most reaction-transport models offer less than 3-D flow fields, have limited capabilities for introducing heterogeneities in the flow regime, and tend to consider only static boundary conditions.

Computer codes typically are used to perform numerical algorithms that model chemical reactivity, hydrochemical transport, and in some cases both. Factors associated with choosing among forward, inverse, and reaction-transport modeling depend on the nature of the geochemical system being considered. Forward modeling may be preferred when only the final outcome of the interaction of groundwater with soils or sediments is desired, i.e., groundwater composition and mineral saturation index. Inverse modeling provides hydrologic information about an aquifer, such as net mass transfer and mixing, and can be used to determine relative rates of reactions.

Most models allow testing only to see if expected reactions occur to a significant or insignificant extent along a designated flowpath. However, one code (EQ3/EQ6) incorporates reaction rate constants.

Another comparison may be made in which forward modeling tests the validity of suspected reactions based on thermodynamic considerations, whereas inverse modeling tests their feasibility based on mass balance considerations. Reaction-transport modeling is distinct, in that it can be used to simulate real transport processes, such as advection and dispersion, in addition to predicting groundwater chemistry. Thus, reaction-transport models may be especially useful for predicting the flowpath of both conservative and nonconservative species.

The availability of data is also a consideration in selecting a geochemical modeling code. Generally, fewer data are needed in forward modeling, whereas fairly complete data are required to achieve definitive results by inverse modeling. As with forward modeling, reaction-transport models may be run with limited chemical data; however, in addition the hydraulic properties of the flow system must be understood.

Not only has it been difficult to use geochemical codes to quantitatively predict the amount of precipitate generated, it is unclear how such a prediction could be correlated to porosity losses and reduced hydraulic conductivity in the reactive cell. Many precipitates could be fine enough to be transported out of the reactive cell through colloidal transport. Therefore, at many permeable sites in the past, a qualitative evaluation of the inorganic data has been used to estimate the potential for precipitate formation in the reactive cell. Site characterization usually gives the first indication. If alkalinity is low or total dissolved solids are high in the groundwater, there is higher potential for precipitates to develop. Selection of appropriate reactive media can alleviate this propensity. After column tests are conducted, changes in dissolved calcium, iron, and alkalinity between column influent and effluent samples can be examined to evaluate the potential for carbonate or hydroxide precipitation.

In general, designers have been satisfied with classifying a site as having either *low* or *high* potential for precipitate formation. An appropriate reactive medium (e.g, iron-pyrite mixture for high-precipitation-potential sites) may then be identified. Greater or lesser safety factors can also be incorporated into the hydraulic design of the permeable barrier according to the type of site. For example, a coarser reactive medium particle size or other method to obtain a higher installed K_{cell} could be incorporated into the design to account for future porosity losses at a high-precipitation-potential site.